

Computational mechanics of material interfaces: trends & challenges

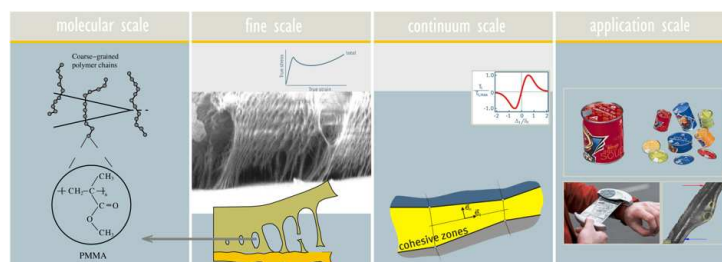
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Interfaces are omnipresent in most engineering materials and structures across the scales, and they have a major impact on the resulting mechanical properties, both in the positive and the negative sense. Considerable research efforts are nowadays focused on the adequate computational description of the interface, which has to account for its different constitutive behaviour modes at each of the scales. At the level of micro-scale deformation mechanisms these modes typically are: constraining deformation (hard surface coatings, interfaces in precipitation strengthened alloys), absorbing deformation (decohesion and delamination), transmitting deformation (plastic slip through grain boundaries). The role of external and internal boundaries is even more dominant in micromechanical systems, where the surface-to-volume ratio changes drastically. Ample research efforts are being initiated in the field to reveal the mechanical behaviour of interfaces and surfaces across the scales, whereby the computational modelling thereof is a prime goal.

This presentation addresses trends and challenges in the computational mechanics modelling of interfaces, from different perspectives:

- *Cohesive zones*: They are by now a classical tool to describe one of the particular behaviour modes of interfaces, dominated by decohesion and delamination. In the context of this wide spread field of computational mechanics, emphasis is put on two particular issues:
 - Large deformation description: unlike solids and fluids, this has received less attention for cohesive zones. The problem will be addressed with a delamination example revealing very large deformations.
 - Quasi-brittle interfaces: it is known that the cohesive zone modelling of brittle delamination processes suffers from an extreme discretization sensitivity. To remedy this problem, a enriched cohesive zone element will be presented.
- *Intrinsic multi-scale aspects*: The cohesive zone concept lumps all deformation in the interfacial decohesion plane. The limitations thereof are not always properly understood, and will be illustrated with a particular example. These limitations call for an extended interfacial description, in which novel multi-scale methods play an important role.



Multi-scale characterization of delaminating polymer-metal interfaces

- *Constraining interfaces*: Compatible interfaces will naturally induce a constraint through the coarse-scale elastic fields. Less obvious are the resulting constraints acting on the micro-scale carriers of deformation and the resulting coarse grained impact thereof. This holds particularly for plastic slip in metals, as occurring at grain boundaries, phase boundaries, oxide layers, coatings, etc. This problem reveals the intrinsic role of discreteness and shows a rigorous link with strain gradient plasticity models, whereby its physical justification becomes more natural.
- *Transmitting interfaces*: In some particular cases, fine scale deformation carriers are able to cross the interface. This is particularly relevant for interfaces joining materials with similar atomic or microstructures and similar deformation carriers, e.g. dislocation-based slip in single phase or multi-phase polycrystals. A simple grain boundary is the most typical example, and proper constitutive equations to describe the physical phenomena accurately are still lacking.
- *Interfaces in micro-electronics and miniaturized systems*: Interfaces and boundaries in micro-electronics and miniaturized systems are intrinsically important, for which the typical size of the material's microstructure is no longer negligible with respect to the component or structural size. As a result, typical failure modes and a number of characteristic size effects emerge.
- *Multi-physics aspects of interfaces in solids*: There are several engineering problems, which are characterized by the intrinsic interaction between the mechanical field and other fields acting through the interface (e.g. thermo-mechanical interaction in heat conduction, electro-mechanical interaction in MEMS, etc.). Challenges in this context are given on the basis of a practical example, i.e. thermoshock damage in a refractory material.

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